

Correlation Effect on Peierls Transition

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The effect of correlation on Peierls transition, which is accompanied by a dimerization, t_d , of a bond alternation for transfer energy, has been examined for a half-filled one-dimensional electron system with on-site repulsive interaction (U). By applying the renormalization group method to the interaction of the bosonized Hamiltonian, the dimerization has been calculated variationally and self-consistently with a fixed electron-phonon coupling constant (λ) and it is shown that t_d takes a maximum as a function of U . The result is examined in terms of charge gap and spin gap and is compared with that of the numerical simulation by Hirsch [Phys. Rev. Lett **51** (1983) 296]. Relevance to the spin Peierls transition in organic conductors is discussed.

KEYWORDS: Peierls transition, Hubbard model, dimerization, renormalization, charge gap, spin gap

Peierls transition for a one-dimensional half-filled electron system coupled with phonon has been studied extensively since the Su-Schrieffer-Heeger model was proposed for the quasi-one-dimensional conductor polyacetylene with a bond alternation.¹⁾ The role of correlation in such a model has been examined by introducing an on-site repulsive interaction, U . The calculation using the Hartree-Fock approximation leads to the Peierls state, which exists only for U smaller than a critical value of the order of the band width.^{2,3)} This study has been further developed by taking into account a one-dimensional quantum fluctuation. The numerical simulation exhibits an enhancement of dimerization in the presence of repulsive interaction.^{4,5,6,7,8,9)} A notable finding is that the dimerization takes a maximum at a value of U being nearly the band width^{5,8,9)} and that the charge gap becomes much larger than the dimerization gap.⁵⁾ Regarding the case of weak coupling, the analytical method of a renormalization group (RG) has also exhibited the enhancement of t_d as a function of U .¹⁰⁾ The effect of finite phonon frequency has been explored using the RG method based on the bosonization.^{11,12,13)} It has been shown that the half-filled case leads to a competition between the state with both spin and charge gaps and the state with only a charge gap on the plane of the phonon frequency and the electron-phonon coupling constant.¹³⁾ In contrast, the case of strong coupling with large U has been examined in terms of the opposite approach, i.e., the expansion of $1/U$ and mapping the electron system into a spin 1/2 chain system, which leads to the spin Peierls transition. The successful treatment of the quantum fluctuation leads to the occurrence of the spin Peierls transition for an arbitrary magnitude of the electron-phonon coupling constant.^{14,15,16)} However, it is not clear why the optimum condition for the Peierls transition is given by the intermediate coupling of U .

In the present paper, the unconventional role of U on

the Peierls state is examined by applying the RG method to the bosonized Hamiltonian. It is demonstrated that a maximum of the dimerization occurs for $U \simeq 2t$ ($4t$ is the band width) for weak electron-phonon coupling (λ), and that the charge gap is well separated from the spin gap at the maximum. Furthermore, we discuss the relevance of this to the spin Peierls transition in an organic conductor, (TMTTF)₂PF₆ salt.^{17,18)}

We consider a one-dimensional half-filled Hamiltonian given by^{1,2,3)}

$$H = \sum_j \left[- \sum_{\sigma} (t - (-1)^j t_d) (c_{j,\sigma}^{\dagger} c_{j+1,\sigma} + h.c.) + U n_{j,\uparrow} n_{j,\downarrow} + C t_d^2 / 2 \right], \quad (1)$$

where $c_{j,\sigma}^{\dagger}$ denotes a creation operator of a conduction electron with spin σ ($=\uparrow, \downarrow$) at the lattice site j . The first term is the kinetic energy, where t is the uniform transfer energy. The quantity, t_d , which denotes the dimerization due to Peierls distortion, is determined so as to minimize the total energy. The U term with $n_{j,\sigma} = c_{j,\sigma}^{\dagger} c_{j,\sigma}$ denotes an on-site repulsive interaction, and the last term with a constant C is the elastic energy for the distortion.

Applying the bosonization method,^{19,20)} eq.(1) for the half-filled case is rewritten as

$$H = + \frac{v_{\rho}}{4\pi} \int dx \left[\frac{1}{K_{\rho}} (\partial_x \theta_+)^2 + K_{\rho} (\partial_x \theta_-)^2 \right] + \frac{v_{\sigma}}{4\pi} \int dx \left[\frac{1}{K_{\sigma}} (\partial_x \phi_+)^2 + K_{\sigma} (\partial_x \phi_-)^2 \right] + \frac{v_F}{2\pi\alpha^2} \int dx \left[y_{1/2} \cos 2\theta_+ + y_{\sigma} \cos 2\phi_+ - y_W \sin \theta_+ \cos \phi_+ + (1/8\lambda) y_W^2 \right], \quad (2)$$

where $\theta_{\pm}(x)$ and $\phi_{\pm}(x)$ denote phase variables for the charge and spin fluctuation, respectively,²¹⁾ and $[\theta_+(x), \theta_-(x')] = [\phi_+(x), \phi_-(x')] = i\pi \operatorname{sgn}(x - x')$.

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The $y_{1/2}$ term and the y_W term represent the Umklapp scattering and the dimerization, respectively. The coefficients in eq.(2) are given by $K_\rho = (1 + \tilde{U})^{-1/2}$, $K_\sigma = (1 - \tilde{U})^{-1/2}$, $v_\rho = v_F(1 + \tilde{U})^{1/2}$, $v_\sigma = v_F(1 - \tilde{U})^{1/2}$, $y_{1/2} = y_\sigma = \tilde{U}$, $y_W = 8\alpha t_d/v_F$, $1/\lambda = \pi v_F C/8a$, $v_F = 2ta \sin k_F a (= 2ta)$, $k_F = \pi/(2a)$ and $\tilde{U} = Ua/(\pi v_F)$. The quantity α is a cutoff parameter of the order of the lattice constant, a ; the ratio of α to a will be evaluated later. The quantity y_W is determined by minimizing the total energy, and the resultant self-consistency equation is written as

$$\frac{1}{4\lambda} y_W = \langle \sin \theta_+ \cos \phi_+ \rangle (\equiv \Delta), \quad (3)$$

where $y_W = 4t_d\alpha/(ta)$. The quantity Δ , which denotes an order parameter for the dimerization, is calculated self-consistently in terms of eq.(2). Equation (2) is examined using the RG method with a scaling $\alpha \rightarrow \alpha(1 + dl)$. Within the lowest order of perturbation, RG equations for the coupling constants are derived as^{22,23,11,12,13,24)}

$$\begin{aligned} \frac{d}{dl} K_\rho(l) &= -\frac{1}{2} y_{1/2}^2(l) K_\rho^2(l) - \frac{1}{16} y_W^2(l) K_\rho^2(l), \\ \frac{d}{dl} G_\sigma(l) &= -y_\sigma^2(l) - \frac{1}{8} y_W^2(l), \\ \frac{d}{dl} y_{1/2}(l) &= [2 - 2K_\rho(l)] y_{1/2}(l) + \frac{1}{8} y_W^2(l), \\ \frac{d}{dl} y_\sigma(l) &= -G_\sigma(l) y_\sigma(l) - \frac{1}{8} y_W^2(l), \\ \frac{d}{dl} y_W(l) &= \left[\frac{3}{2} - \frac{1}{2} K_\rho(l) - \frac{1}{4} G_\sigma(l) \right] y_W(l) \\ &\quad + \frac{1}{2} y_{1/2}(l) y_W(l) - \frac{1}{2} y_\sigma(l) y_W(l), \end{aligned} \quad (4)$$

where $G_\sigma(l) = 2(K_\sigma(l) - 1)$ and initial values at $l = 0$ are given by coefficients of eq.(2). The relevance of $y_{1/2}$, y_σ and y_W corresponds to the appearance of charge gap, spin gap and dimerization, respectively.

For calculating the r.h.s. of eq.(3), we use the fact that the derivative of $\langle \sin \theta_+ \cos \phi_+ \rangle$ with respect to y_W can be expressed in terms of the response function given by

$$R(|\vec{r}_1 - \vec{r}_2|) = \langle T_\tau O_d(\vec{r}_1) O_d(\vec{r}_2) \rangle, \quad (5)$$

where $O_d(\vec{r}) (\equiv \sin \theta_+(\vec{r}) \cos \phi_+(\vec{r}) = -(\pi\alpha/4a) \sum_\sigma (-1)^j c_{j,\sigma}^\dagger c_{j,\sigma} + \text{h.c.})$ denotes an operator for dimerization. The vector \vec{r} consists of space $x (= ja)$ and imaginary time τ while T_τ is the time-ordering operator. Using the RG method, $R(t_d, l) (= R(|\vec{r}|))$ is calculated as²⁵⁾

$$\begin{aligned} R(t_d, l) &= \frac{1}{4} \exp \left[- \int_0^l dl' (K_\rho(l') \right. \\ &\quad \left. + K_\sigma(l') - y_{1/2}(l') + y_\sigma(l')) \right], \quad (l \leq l_c) \\ R(t_d, l) &= \frac{1}{4} \exp \left[- \int_0^{l_c} dl' (K_\rho(l') \right. \\ &\quad \left. + K_\sigma(l') - y_{1/2}(l') + y_\sigma(l')) \right] \\ &\quad \times \exp \left[- \int_{l_c}^l dl' (K_\sigma(l') + y_\sigma(l')) \right], \quad (l > l_c) \end{aligned} \quad (6)$$

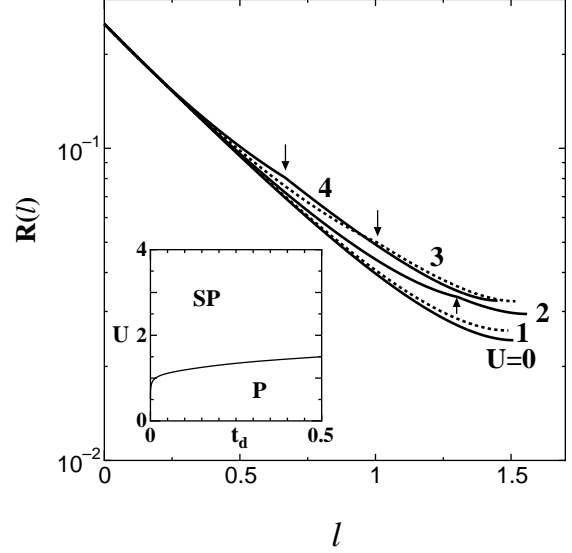


Fig. 1. l -dependence of $R(l)$ of eq.(6) for $t_d = 0.1$, and $U = 0, 1, 2, 3$ and 4 where $R(l)$ decreases and takes a minimum at $l = l_m$. $t = 1$ and $\alpha/a = 1.52$. The arrow denotes $l = l_c$ given by $y_{1/2}(l_c) = 1$. In the inset, the spin Peierls (SP) region and the Peierls (P) region correspond to $l_c < l_m$ and $l_c > l_m$, respectively, where the boundary denotes a crossover between these two regions.

where $l = \ln([x^2 + (v_F\tau)^2]^{1/2}/\alpha)$. In eq.(6), we introduced $l = l_c$ with $y_{1/2}(l_c) = 1$, from which the charge gap is calculated. The response function for $l > l_c$ is calculated by estimating $\langle \sin \theta_+ \rangle$ in the presence of the charge gap. Although one expects $R(\infty) \rightarrow \Delta^2$, we use the following method to estimate Δ within the present RG equation, which leads to $R(l)$ taking a minimum at $l = l_m$. Since $R(l)$ as a function of l becomes invalid for $l > l_m$, we use a self-consistency equation for $\Delta (= \Delta(t_d))$ given by

$$\Delta(t_d) = \int_0^{t_d} dt'_d \int_0^{l_m(t'_d)} dl' e^{2l'} \{ R(t'_d, l') - \Delta^2(t'_d) \} \quad (7)$$

We assume $t = 1$ in the following numerical calculation, if there is no confusion. For estimating the r.h.s. of eq.(7), we calculate RG eq.(4). When l increases with fixed U , one finds the decrease of $K_\rho(l)$, $G_\sigma(l)$ and $y_\sigma(l)$ and the increase of $y_{1/2}$ and y_W . Behaviors at large l are classified into two groups depending on the magnitude of $y_W(0)$. For small $y_W(0)$, $y_{1/2}(l)$ is larger than $y_W(l)$, while $y_{1/2}(l)$ becomes smaller than $y_W(l)$ with increasing $y_W(0)$. The former case denotes the Peierls state in the presence of a well-developed charge gap since the relevance of $y_{1/2}$ (y_W) corresponds to the formation of the charge gap (the formation of both charge and spin gaps due to the Peierls distortion).

The response function is calculated by substituting the solution of RG equations into eq.(6). In Fig.1, the l -dependence of $R(l)$ is shown for $t_d = 0.1$ and certain values of U . The results are shown in the region with $l < l_m$, where $R(l_m)$ is a minimum of $R(l)$. The long range order of the Peierls state is related to the relevance of y_W , which leads to the appearance of l_m in the present approximation of the RG equations. The arrow

for $U = 2, 3$ and 4 denotes the location at $l = l_c$ where $y_{1/2}(l_c) = 1$. From a comparison of l_c with l_m , one finds a distinction between case I ($l_m > l_c$) and case II ($l_m < l_c$). The charge gap is already developed prior to obtaining the Peierls state in case I. The inset depicts the spin Peierls region (case I) and the Peierls region (case II) on the plane of U and t_d . The charge gap dominates for $U \gtrsim 1.5$ and $t_d < 0.5$. The solid curve shows the boundary as a crossover between these two regions, where the state moves continuously.

An estimation of the ratio of α/a is needed for the calculation of Δ of eq.(7) as a function of t_d and U . When $U = 0$, Δ becomes equal to the order parameter of the conventional Peierls distortion and thus the r.h.s. of eq.(3) can be calculated rigorously as $\Delta \rightarrow \Delta_{\text{Peierls}} = (t_d \alpha/a) \int_0^\pi dz (\sin z)^2 / [(2 \cos z)^2 + (2 t_d \sin z)^2]^{1/2}$, which leads to $(t_d \alpha/a) \times \ln(1.4/t_d)$ for small t_d . By comparing Δ_{Peierls} with that obtained from eq.(7), we obtain $\alpha/a \simeq 1.5 \pm 0.02$ for small t_d ($\lesssim 0.2$).

In terms of the response function, Δ is calculated self-

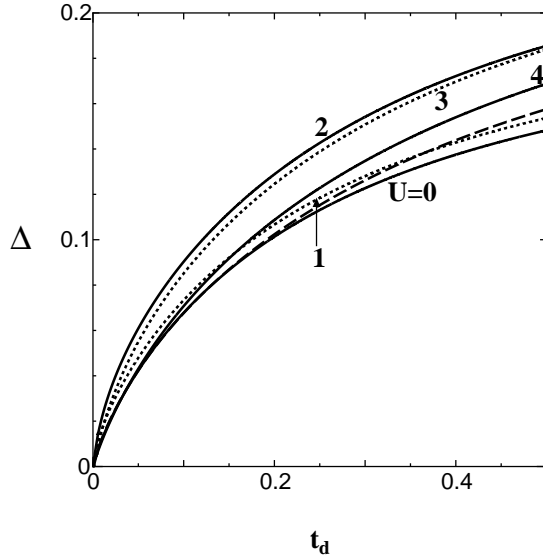


Fig. 2. t_d -dependence of Δ calculated self-consistently by using eq.(7) for $U = 0, 1, 2, 3$ and 4 . The dashed curve denotes Δ_{Peierls} .

consistently from eq. (7). In Fig. 2, Δ is shown as a function of t_d for certain values of U . The dashed curve denotes Δ_{Peierls} which coincides well with that of $U = 0$ (solid curve) for $t_d \lesssim 0.2$. With increasing t_d , Δ for fixed U increases monotonically. The self-consistent result of Δ obtained from eq. (7) is smaller than $R(l_m)^{1/2}$, e.g., $\Delta/R(l_m)^{1/2} = 0.43, 0.45, 0.52, 0.47$ and 0.39 for $U = 0, 1, 2, 3$ and 4 . This is reasonable since the lowest order RG equation with the relevant coupling overestimates the response function for large l . From the comparison of Δ for $U = 2$ with that for $U = 3$, it is found that Δ as a function of U ($\gtrsim 2$) decreases, indicating the existence of an optimum value of U for the Peierls state.

Based on Fig. 2, we obtain the dimerization, t_d , representing the Peierls state, which is calculated using eq.(3). In Fig. 3, t_d is shown as a function of λ with certain values of U . The dashed curve denotes $t_d (\simeq 1.4 \exp[-1/\lambda])$

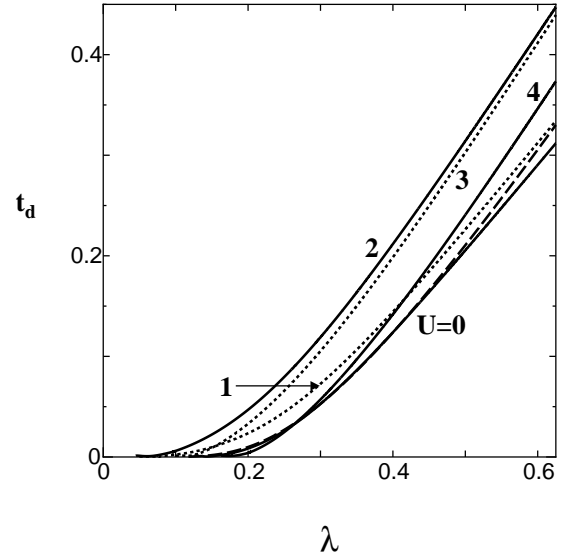


Fig. 3. λ -dependence of t_d , which is calculated from eq.(3), for $U = 0, 1, 2, 3$ and 4 where the dashed curve denotes Δ_{Peierls} corresponding to the conventional calculation in the absence of U .

obtained from Δ_{Peierls} , which coincides with t_d in the case of $U = 0$ (solid curve) for $0.25 \lesssim \lambda \lesssim 0.5$ within the visible scale. For small λ , t_d decreases exponentially but is enhanced sufficiently for $U = 1, 2$ and 3 . We note that t_d takes a maximum around $U \simeq 2$. Such a U -dependence of t_d , indicating a crossover from the regime of weak coupling to that of strong coupling, is elucidated by examining the relevant term of $y_W \sin \theta_+ \cos \phi_+$ in eq.(2) and the corresponding RG equation (the last equation of eq.(4)). For small U , the y_W -term is enhanced by the Umklapp scattering of the $y_{1/2}$ -term, which leads to the suppression of charge fluctuation (θ_+). For large U , both y_σ and K_σ increase the quantum fluctuation for the spin part (ϕ_+) resulting in the suppression of $\langle \cos \phi_+ \rangle$ for the Peierls state.

The U -dependence of $t_d (= \Delta \lambda a / \alpha)$ is obtained by examining t_d with fixed λ in Fig. 3. In Fig. 4, t_d with $\lambda = 0.25$ is depicted as a function of U by the solid curve. As expected from Fig. 2 and Fig.3, t_d takes a maximum around $U = 2$. The triangle, which represents the numerical result obtained by Hirsch,⁵⁾ is compared with the dashed curve of the present calculation with $\lambda = 0.42$ (dashed curve) corresponding to the parameter of the numerical simulation. The fact that the dashed curve is larger than the numerical result (triangle) is reasonable since the present calculation treats the dimerization (the bond alternation) classically while the numerical simulation has been performed in the presence of the quantum fluctuation. We note that there is not much variation of the location of U for the maximum, e.g., the maximum appears at $U = 2.2 \pm 0.1$ in the interval range of $0.2 \lesssim \lambda \lesssim 0.5$. In the inset, the U -dependences of the charge gap (Δ_ρ) and spin gap (Δ_σ) for $\lambda = 0.25$ are shown by a solid curve and dotted curve, respectively. These gaps are calculated by $\Delta_\rho / \omega_c = \exp[-l_c]$ and $\Delta_\sigma / \omega_c = \exp[-l_\sigma]$ with $|y_\sigma(l_\sigma)| = 1$, where $\omega_c (\simeq 2.37)$

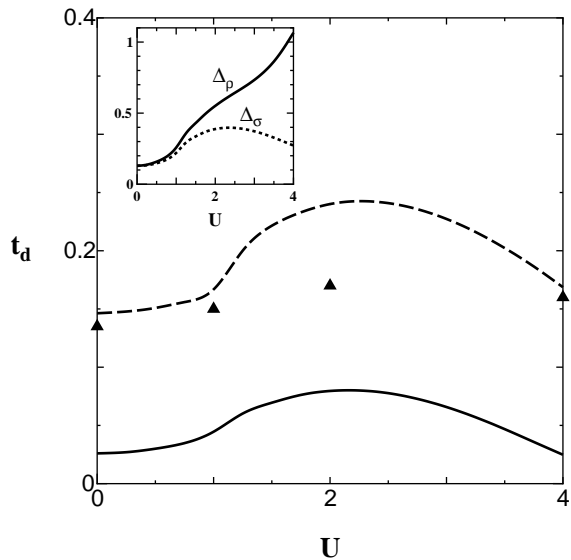


Fig. 4. Quantity t_d as a function of U for $\lambda = 0.25$ (solid curve). The symbol (triangle) is the result calculated by Hirsch,⁵⁾ which is compared with the present calculation with $\lambda = 0.42$. The inset shows the charge gap (Δ_ρ) and the spin gap (Δ_σ) for $\lambda = 0.25$.

is chosen so as to obtain Δ_ρ with $t_d = 0$ nearly equal to the well-known exact one. With increasing U , Δ_ρ increases monotonically while Δ_σ takes a maximum. The maximum of t_d is found to be accompanied by the separation of charge gap and spin gap. Thus, it is expected that with increasing U , there is a crossover from the conventional Peierls state with $\Delta_\rho \simeq \Delta_\sigma$ to the spin Peierls state with the charge gap being much larger than the spin gap.

When U is extremely large, the effect of t_d can be examined using the bosonized phase Hamiltonian of spin 1/2 chain¹⁶⁾ with the antiferromagnetic exchange energy, $4(t \pm t_d)^2/U$. The calculation of t_d , similar to eq.(3), with only a spin degree of freedom shows that t_d decreases monotonically with increasing U . From comparison of the present result with this limiting one (not shown explicitly), the present calculation for $U \lesssim 4$ in Fig. 3 seems to be reasonably extrapolated to that of the spin 1/2 chain except for small t_d (and then small λ), which requires much accuracy of numerical evaluation.

Finally, we discuss the spin Peierls transition in an organic conductor, (TMTTF)₂PF₆, which has been observed by magnetic and X-ray experiments.^{26,27)} This conductor, which indicates the charge gap being much larger than the spin gap¹⁸⁾ is often analyzed in terms of a model with spin 1/2 chain although U is of the order of the band width.²⁸⁾ The conductor has a quarter-filled band with a dimerization, which may be considered to be half-filling. However, such an effectively half-filled band strongly reduces the magnitude of Umklapp scattering, resulting in the suppression of the Peierls state. In fact, the Umklapp scattering is estimated to be $y_{1/2} = 2(x_d/(1+x_d^2))\tilde{U}$, where $v_F = \sqrt{2}ta$ and x_d corresponds to a dimerization for a quarter-filling.²⁹⁾ For $x_d \simeq 0.1$ corresponding to TMTTF salt,¹⁷⁾ we find that t_d as a function

of U decreases for small U while separation between Δ_ρ and Δ_σ appears for $U \gtrsim 3$. Moreover, with decreasing x_d and fixed λ ($\lesssim 0.5$), t_d decreases strongly for $U = 4 \sim 6$. When $U = 5.6$ and $\lambda = 0.25(0.5)$, we obtain the dimerization as $t_d = 0.036(0.23)$, $0.019(0.17)$ and $\simeq 0(0.05)$; the charge gap as $\Delta_\rho = 0.31(1.05)$, $0.12(0.73)$ and $\simeq 0(0.17)$; the spin gap as $\Delta_\sigma = 0.18(0.77)$, $0.08(0.57)$ and $\simeq 0(0.15)$, for $x_d = 0.2, 0.1$ and 0 , respectively. Based on such a consideration, the spin Peierls state in the organic conductor could be realized when Umklapp scattering induced by the electronic correlation becomes large.

In summary, we have examined the effect of on-site repulsive interaction, U , on the Peierls state with dimerization t_d . For small (large) U , t_d increases (decreases) where the charge gap is almost equal to (much larger than) the spin gap. The maximum of t_d indicates a crossover from the weak coupling regime, in which the Umklapp scattering suppresses the charge fluctuation, into a strong coupling regime, in which the quantum spin fluctuation reduces the effect of dimerization.

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